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研究论文

丙烯腈在Cu(111)面上化学吸附的密度泛函研究及NBO分析

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摘要 利用密度泛函方法对丙烯腈在Cu(111)面上不同吸附位的吸附状态进行了理论研究. 计算结果表明, 丙烯腈分子通过端位N原子立式吸附在金属铜表面为弱化学吸附, 其中桥位为较佳吸附位, 结合能为-40.16 kJ/mol; 丙烯腈分子和金属铜之间发生了电荷转移, N原子的孤对电子与金属形成σ共价键; 对丙烯腈分子结构变化进行了NBO分析, 解释了丙烯腈分子吸附后被活化的原因.

关键词 密度泛函 丙烯腈 Cu(111) 化学吸附 自然键轨道

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DFT Study and NBO Analysis of Chemisorption of Acrylonitile on Cu(111)

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Abstract Adsorption of acrylonitrile(AN) on different sites of Cu(111) surface was studied by using model copper cluster Cu_{16} with density functional theory (DFT). AN adsorbed perpendicularly to the surface and bonded to the metal sites *via* a nitrogen-metal interaction, *i.e.*, a weak chemisorption. Such chemisorption led to electron transfer between the AN molecule and the cluster. In complexes Cu_{16}—AN, the σ-binding *via* the lone-pair electrons of N atom and Cu atom was observed. Adsorption on bridge site was preferred with binding energy of 40.16 kJ/mol. The backbone of AN changes a lot due to adsorption, which can be indicated by the variety of bond lengths, bond orders, bond angles, IR spectroscopy and hybridization of chemical bonds. NBO analysis was uesed to explain these changes and why AN was activated by the chemisorption.

Key words Density functional theory; Acrylonitrile; Cu(111) surface; Chemisorption; NBO

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